SAND2012-7265P

DAKOTA 101: Optimization

http://dakota.sandia.gov

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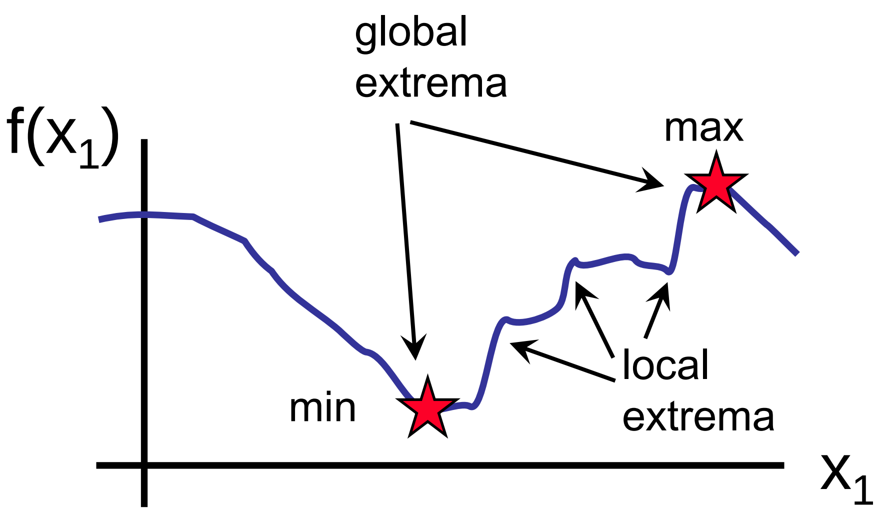
Learning Goals - Optimization

- Define goals of optimization and problem components
- Identify information needed by DAKOTA
- Become familiar with basic solution approaches
- Define optimization problems associated with your field
- Formulate and set up an optimization problem associated with the cantilever beam example
- Find and interpret optimization study results
- Survey problem categories and considerations for method selection

Why Use Optimization?

- What: Determine parameter values that yield extreme values of objectives, while satisfying constraints.
- Why?
  - Identify system designs with maximal performance
    - E.g., case geometry that minimizes drag and weight, yet is sufficiently strong and safe
  - Determine operational settings that maximize system performance
    - E.g., fuel re-loading pattern yielding the smoothest nuclear reactor power distribution while maximizing output
  - Identify minimum-cost system designs/operational settings
    - E.g., delivery network that minimizes cost while also minimizing environmental impact
  - Identify best/worst case scenarios
    - E.g., impact conditions that incur the most damage

Optimization Goals Come in Multiple Forms



Some applications: local improvement suffices; others: must find global minimum at any cost

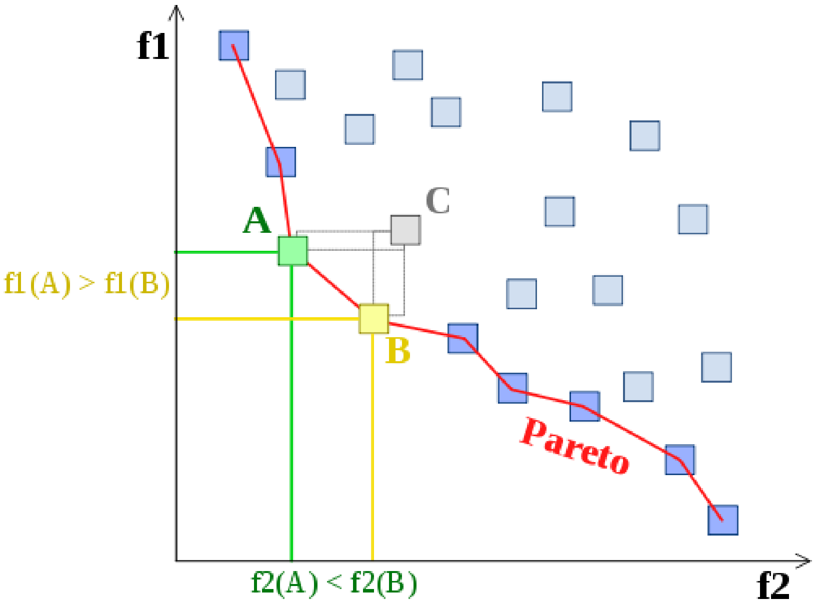
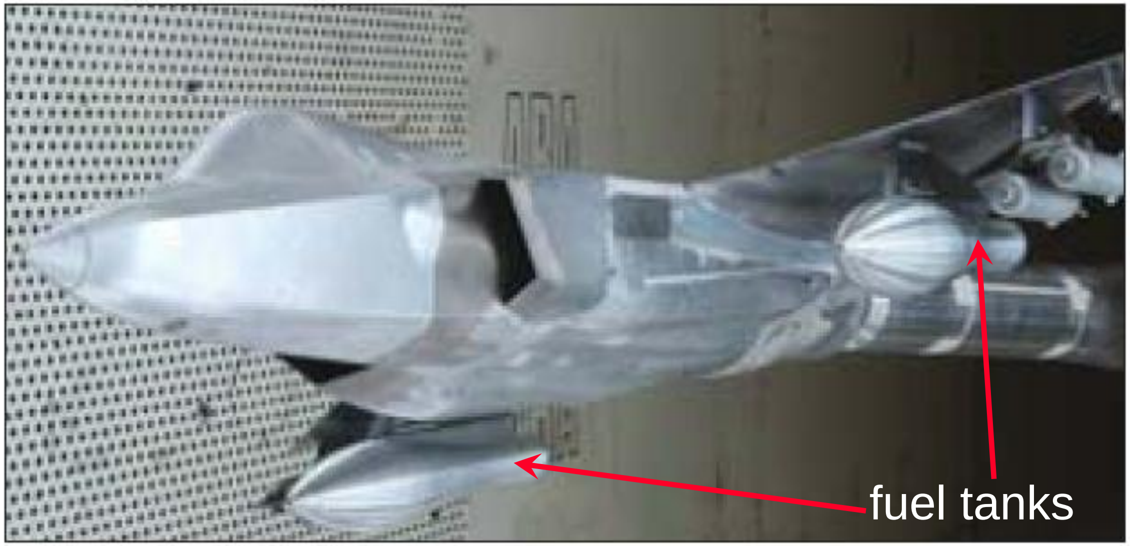


image from
http://en.wikipedia.org/wiki/Pareto_efficiency

May want tradeoffs between multiple objectives

Optimization for Lockheed-Martin F-35 External Fuel Tank Design



This wind tunnel model of F-35 features an optimized external fuel tank.

F-35: stealth and supersonic cruise

~ $20 billion cost

~ 2600 aircraft (USN, USAF, USMC, UK & other foreign buyers)

LM CFD code

- *Expensive*: 8 hrs/job on 16 processors
- Fluid flow around tank *highly sensitive* to shape changes

Optimization Problem

- Goal: Minimize DRAG and YAW over possible values of shape parameters
- Shape parameters must be bounded to fit within prescribed area
- Design must be sufficiently safe and strong

Objective Function: quantity for which we are trying to find the extreme value over parameter ranges

Parameters: quantities to be varied

Constraints: conditions that cannot be violated

Brief Group Discussion: Optimization Practice

5-10 min discussion

- **What types of system design, performance, and cost questions do you ask in your domain?**
- **What metrics do you use to assess design quality, performance level, and costs?**
- **How do you answer your questions currently?**
- **What are the key challenges you face?**
- **Can any of your questions be framed (or re-framed) as finding extremes?**

Anatomy of an Optimization Problem: Mapping to DAKOTA Interface

Computed by simulation and reported to DAKOTA

Minimize:	$f(x_1,\ldots,x_N)$	***Objective function(s)***
Subject to:	$g_{LB} \le g(x) \le g_{UB}$	***Nonlinear inequality constraints***
	$h(x) = h_E$	***Nonlinear equality constraints***
	$A_I x \le b_I$	***Linear inequality constraints***
	$A_E x = b_E$	***Linear equality constraints***
	$x_{LB} \le x \le x_{UB}$	***Bound constraints***

Specified in DAKOTA input file

Anatomy of an Optimization Problem: Mapping to DAKOTA Interface

Need info in "interface" and "responses" blocks

Minimize:	$f(x_1,\ldots,x_N)$	***Objective function(s)***
Subject to:	$g_{LB} \le g(x) \le g_{UB}$	***Nonlinear inequality constraints***
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	$A_E x = b_E$	***Linear equality constraints***
	$x_{LB} \le x \le x_{UB}$	***Bound constraints***

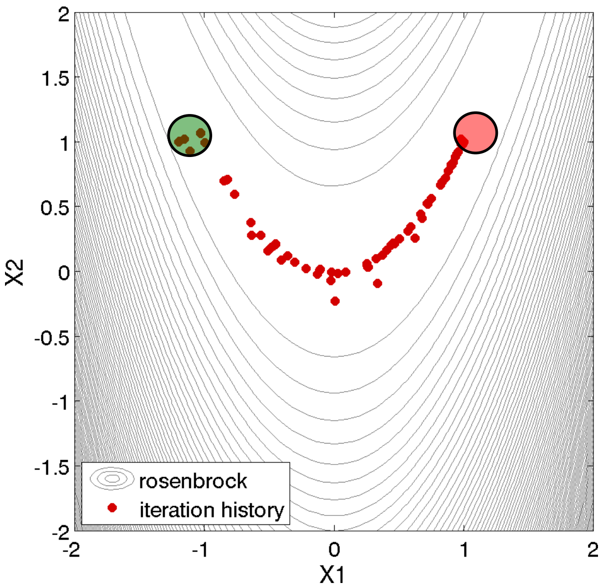
Need info in "method" block

Need info in "variables" block

Basic Classes of Optimization Approaches (the "method" block)

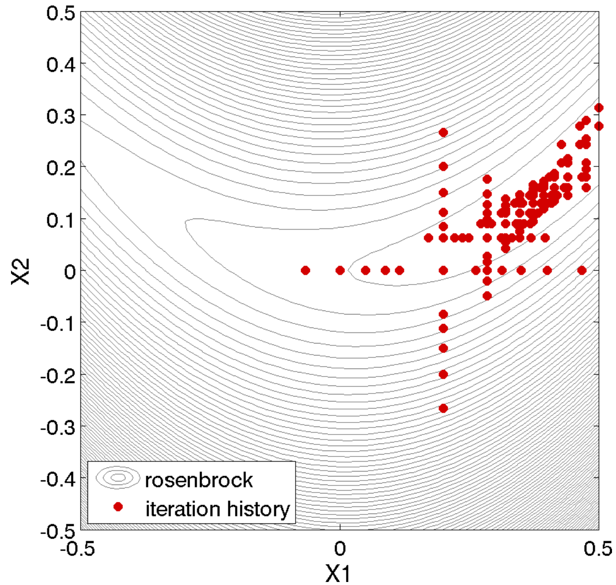
Gradient Descent

- Looks for improvement based on derivative
- Requires analytic or numerical derivatives
- Efficient/scalable for smooth problems
- Converges to local extreme



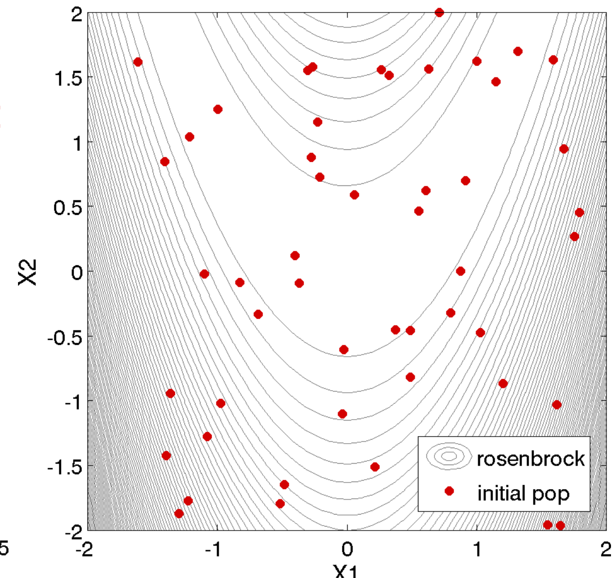
Derivative-Free Local

- Sampling with bias/rules toward improvement
- Requires only function values
- Good for noisy, unreliable or expensive derivatives
- Converges to local extreme

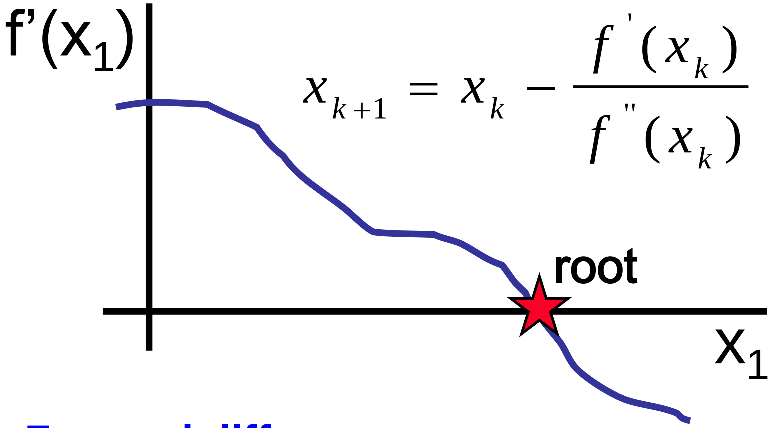


Derivative-Free Global

- Broad exploration with selective exploitation
- Requires only function values
- Typically computationally intensive
- Converges to global extreme



Variations on Gradient-Based Optimizers



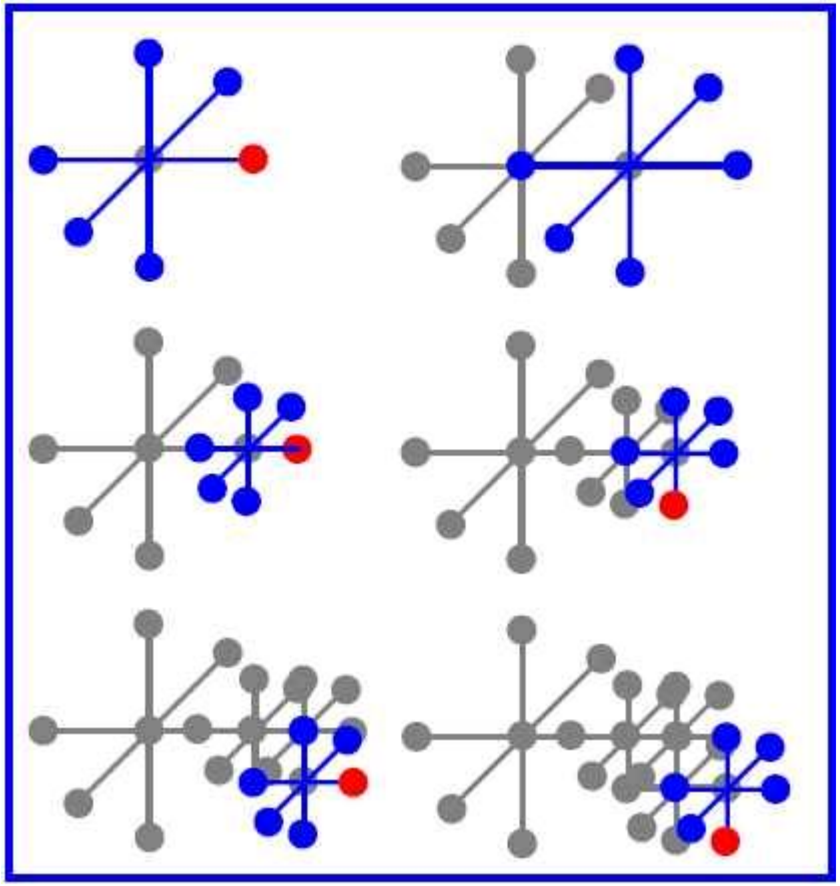
$$x_{k+1} = x_k - \frac{f'(x_k)}{f''(x_k)}$$

Forward difference

$$\frac{\partial f}{\partial x} \approx \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

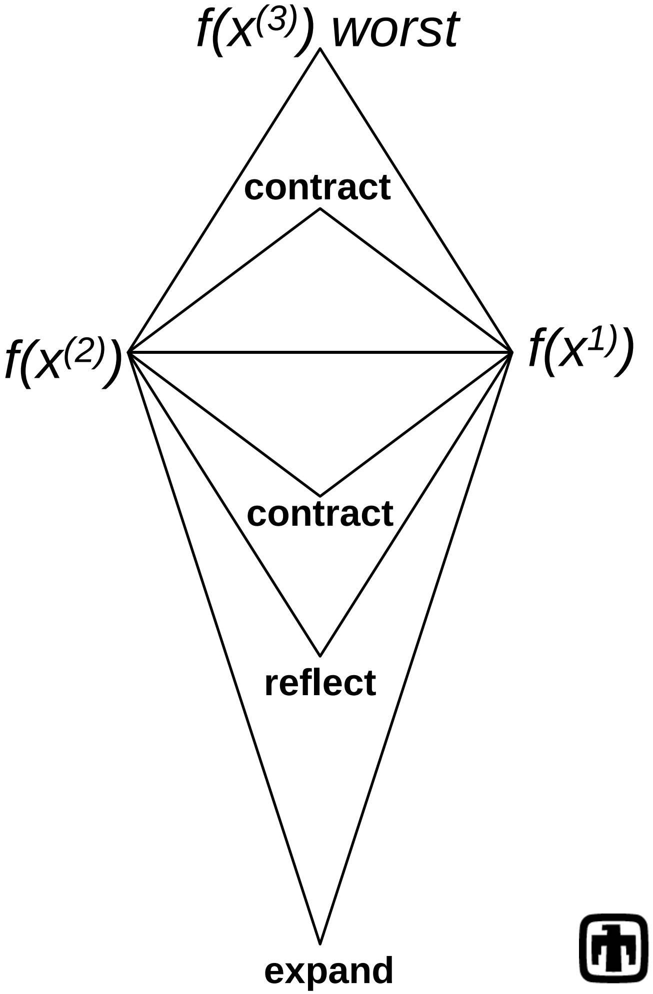
- **Go downhill**
  - **e.g., steepest descent, conjugate gradient, Newton and variants**
  - **second derivatives differentiate minima from maxima, inflection points; Hessian approximations often used in practice (quasi-Newton)**
- **Require reliable derivatives of objectives and nonlinear constraints w.r.t. decision variables:**
  - **analytic evaluation: code them into the simulation**
  - **finite differences: no code modification and provided by most optimizers**
  - **automatic differentiation: source transformation, operator overloading**
- **Strategies for managing convergence:**
  - **line search: find a step in the Newton direction to ensure sufficient decrease**
  - **trust region: use quadratic model in an expanding/contracting trust region**
- **Handling nonlinear constraints**
  - **reduced gradient**
  - **sequential linear or quadratic programming (SLP/SQP)**
  - **augmented Lagrangian or exact penalty methods**
  - **interior point / barrier, filter methods**

Variations on Derivative-Free Optimizers

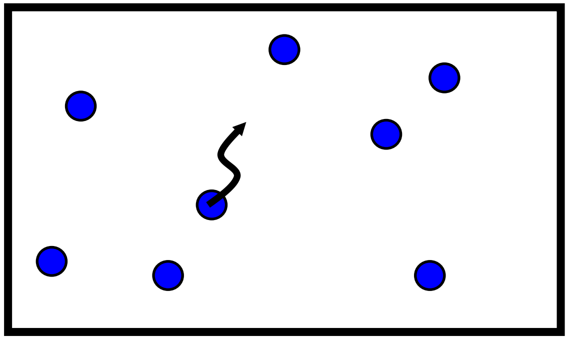


Pattern Search methods search using a stencil, often that defines some basis, that is iteratively re-centered and resized.

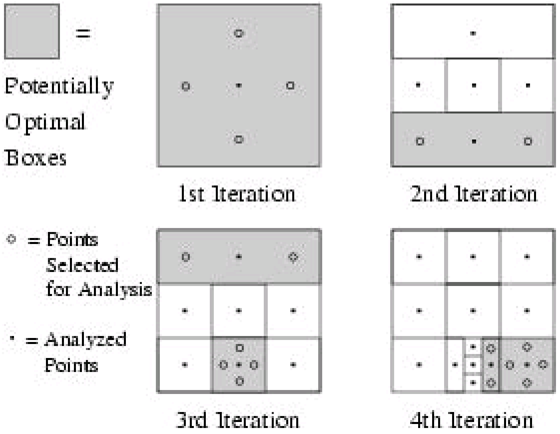
Nelder Mead searches using a simplex that is iteratively reflected through a centroid and resized.



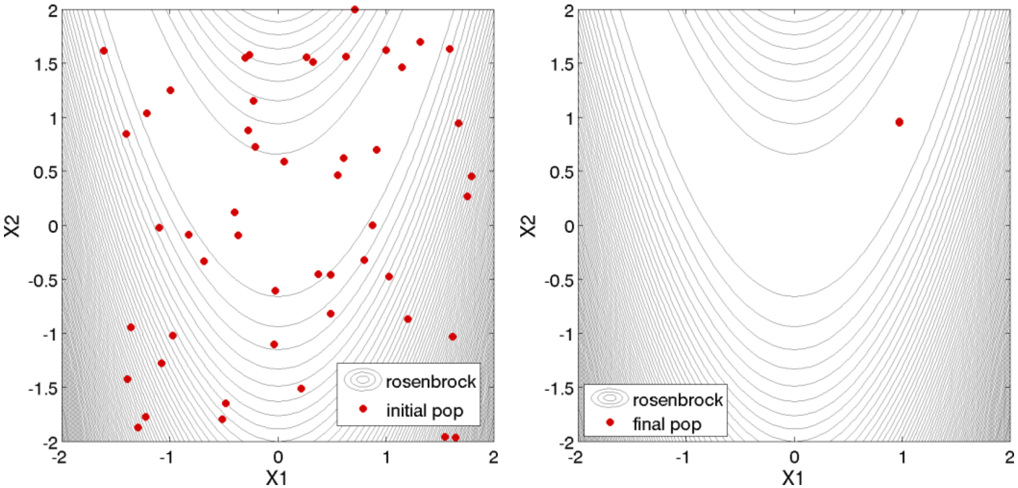
Variations on Global Optimizers



Division of RECTangles (DiRECT) iteratively subdivides the search domain based on size and rank of each existing subdivision.

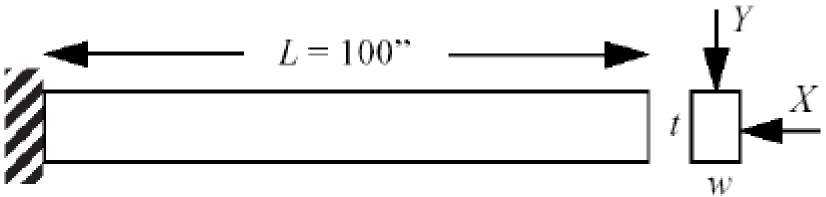


Multi-Start Local Optimization involves initiating a local optimization method at multiple points, with the goal of identifying multiple local minimizers from which the lowest can be chosen.



Evolutionary/Genetic Algorithms evolve an initial random sample over generations, according a "fitness" function, until the minimum is found.

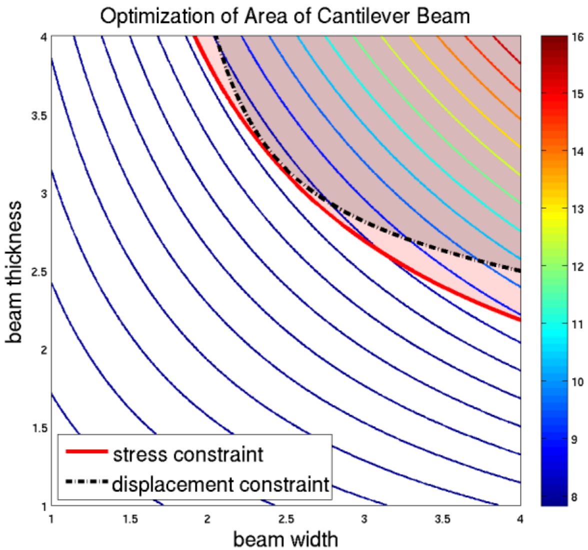
Example Problem:
Cantilever Beam



$$area = w*t$$

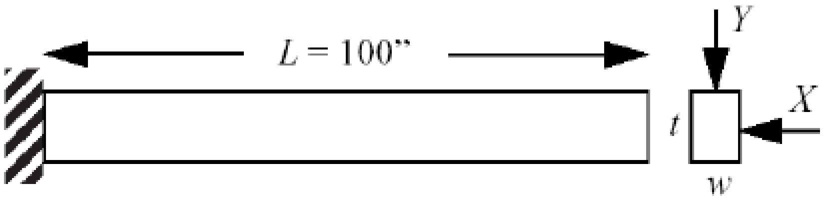
$$stress = \frac{600}{wt^2}Y + \frac{600}{w^2 t}X - R \le 0$$

$$displacement = \frac{4L^3}{Ewt}\sqrt{\left(\frac{Y}{t^2}\right)^2 + \left(\frac{X}{w^2}\right)^2} - D_0 \le 0$$



- **What are some optimal design objectives that may be of interest?**
- **What are some design constraints that may come into play?**
- **What might you expect the results of optimizing a design to be?**

Example Problem:
Cantilever Beam



$$area = w*t$$

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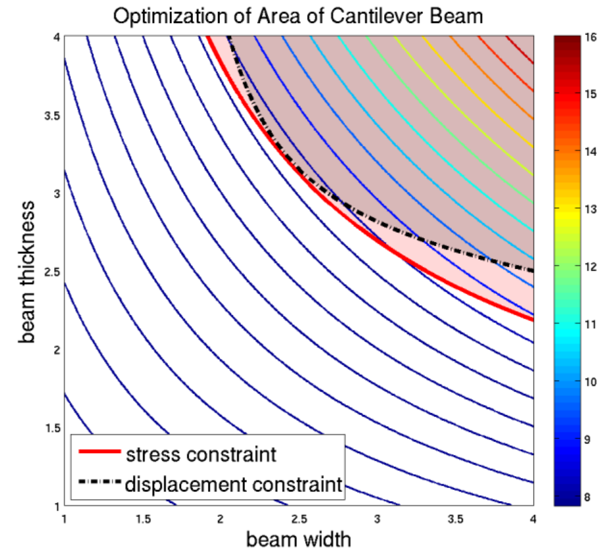

- **Create DAKOTA study to minimize area subject to constraints**
  `1.0 ≤ beam_width ≤ 4.0, 1.0 ≤ beam_thickness ≤ 4.0, stress ≤ 0, displacement ≤ 0`
- **Use nominal (state variables): R=40000, E=2.9e7, X=500, Y=1000**
- **Use CONMIN MFD method (could modify or borrow from template Optimization Local Constrained GradientBased)**
- **Responses: 1 objective (area), 2 nonlinear inequality constraints**
- **Try analytic vs. numerical gradients**
- **Compare to Asynchronous Pattern Search, Coliny EA**

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Potential Solution:
Cantilever Beam Optimization

```
# extraexamples/cantilever_optimization.in
# Perform deterministic optimization with uncertainties at nominal

method
  conmin_mfd

variables
  continuous_design = 2
    upper_bounds    4.0                 4.0
    initial_point   2.5                 2.5
    lower_bounds    1.0                 1.0
    descriptors     'beam_width'        'beam_thickness'
  # Fix at nominal
  continuous_state = 4
    initial_state   40000     2.9e7     500       1000
    descriptors     'R'       'E'       'X'       'Y'

interface
  direct
    analysis_driver = 'mod_cantilever'

responses
  num_objective_functions = 1
  num_nonlinear_inequality_constraints = 2
    descriptors = 'area' 'stress' 'displacement'
  analytic_gradients
  no_hessians
```


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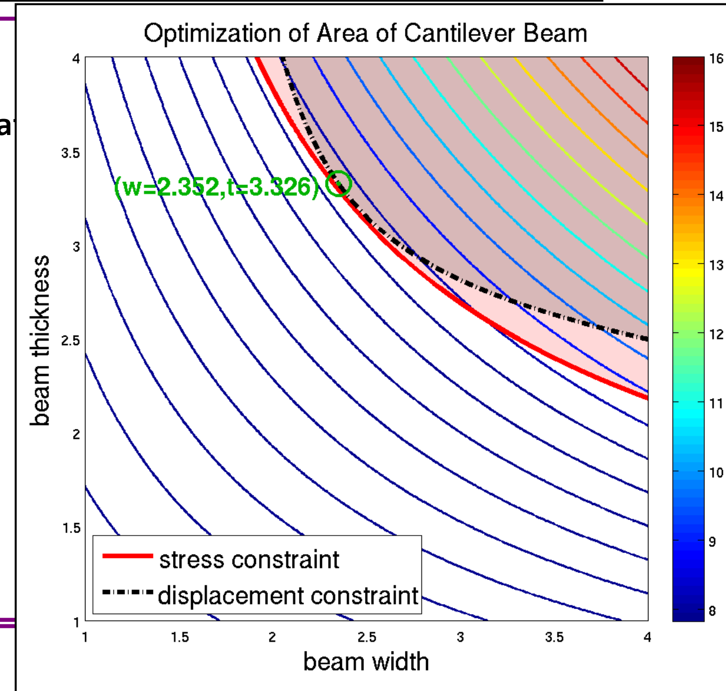
Results:
Cantilever Beam Optimization

```
DAKOTA Standard Output:

<<<<< Function evaluation summary: 93 total (88 new, 5 duplica
<<<<< Best parameters          =
                      2.3518478279e+00 w
                      3.3248865336e+00 t
                      4.0000000000e+04 R
                      2.9000000000e+07 E
                      5.0000000000e+02 X
                      1.0000000000e+03 Y
<<<<< Best objective function  =
                      7.8196271720e+00
<<<<< Best constraint values   =
                     -1.5245380116e-02
                      9.9610350990e-04
```



DAKOTA Tabular Output:

%eval_id	w	t	obj_fn	nln_ineq_con_1	nln_ineq_con_2
1	4	4	16	-0.6484375	-0.7326873741
2	3.8	3.8	14.44	-0.5899548039	-0.6718102213
3	3	3	9	-0.1666666667	-0.1551600958
4	2.840596397	2.840596397	8.068987889	-0.01835621192	0.05104499937
5	2.699999996	2.699999996	7.289999976	0.1431184327	0.2876694251
……………………………					
51	2.354544492	3.321059316	7.819581921	-0.01504188748	0.001014534674
52	2.355218658	3.320102512	7.819567383	-0.01499020104	0.001021619777
53	2.351847828	3.324886534	7.819627172	-0.01524538012	0.0009961035099
54	2.36533115	3.305750446	7.819194503	-0.0141758241	0.001246825701
55	2.363645734	3.308142458	7.819276808	-0.01431664619	0.001193803584

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Brief Group Discussion: Cantilever Problem and Solution

5-10 min discussion

- **Are the results what you expected? Why or why not?**
- **What do you see as the limitations of the method used?**
- **What alternative methods might you try?**

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Optional Examples: Advanced Optimization Problems and Methods

- **Constrained**
  - **Exercise:** Minimize an objective given constraints
- **Multi-start local**
  - **Exercise:** Provide multiple starting points to a local optimizer to find multiple local minima
- **Global**
  - **Exercise:** Find the global extreme value
- **Multi-objective**
  - **Exercise:** Optimize across multiple competing objectives
- **Surrogate-based/multifidelity**
  - **Exercise:** Reduce the computational cost (i.e., number of function evaluations) of optimization
- **Hybrid**
  - **Exercise:** Use multiple optimization methods to solve a single problem

Quick Guide for Optimization Method Selection

Category	DAKOTA method names	Continuous Variables	Categorical/ Discrete Variables	Bound Constraints	General Constraints
Gradient-Based Local (Smooth Response)	`optpp_cg`	x			
	`dot_bfgs, dot_frcg, conmin_frcg`	x		x	
	`npsol_sqp, nlpql_sqp, dot_mmfd, dot_slp, dot_sqp, conmin_mfd, optpp_newton, optpp_q_newton, optpp_fd_newton, weighted sums (multiobjective), pareto_set strategy (multiobjective)`	x		x	x
Gradient-Based Global (Smooth Response)	`hybrid strategy, multi_start strategy`	x		x	x
Derivative-Free Local (Nonsmooth Response)	`optpp_pds`	x		x	
	`asynch_pattern_search, coliny_cobyla, coliny_pattern_search, coliny_solis_wets, surrogate_based_local`	x		x	x
Derivative-Free Global (Nonsmooth Response)	`ncsu_direct`	x		x	
	`coliny_direct, efficient_global, surrogate_based_global`	x		x	x
	`coliny_ea, soga, moga (multiobjective)`	x	x	x	x

See Usage Guidelines in DAKOTA User's Manual

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Optimization References

- J. Nocedal and S. J. Wright, “Numerical Optimization”, Second Edition, Springer Science and Business Media, LLC, New York, New York, 2006.
- S. S. Rao, “Engineering Optimization: Theory and Practice”, Fourth Edition, John Wiley and Sons, Inc., Hoboken, New Jersey, 2009.
- DAKOTA User’s Manual
  - Optimization Capabilities
  - Surrogate-Based Minimization
  - Advanced Strategies
  - Advanced Model Recursions: Optimization Under Uncertainty
- DAKOTA Reference Manual

Learning Goals Revisited: Did we meet them?

- **Define goals of optimization and problem components**
- **Identify information needed by DAKOTA**
- **Become familiar with basic solution approaches**
- **Define optimization problems associated with your field**
- **Formulate and set up an optimization problem associated with the cantilever beam example**
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